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A versatile, refrigerant- and cryogen-free cryofocusing–thermodesorption unit for preconcentration of traces gases in air

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Supplementary Information

Table S-1 shows a list of substances detected up to the time of completion of this paper. Identifications based on ambient air samples as well as synthetic mixtures. Substances are separated into six classes (e.g. CFCs and HCFCs, PFCs and HFCs etc.), which are listed in arbitrary order. Within each class, substances are sorted according to their boiling point (bp) in [°C]. Chemical sum formula as well as retention time t_R in [min] on the GS GasPro PLOT column listed in columns two and three. Columns 5 & 6 show analyte residues in [%], expressed as chromatographic signal area determined in a blank gas measurement relative to a signal area determined in a preceding 1 L ambient air sample. Blank gas: purified helium 6.0 (Praxair, Germany). "Residue HayeSep D" denotes residues found with HayeSep D as adsorptive material, "Residue Unibeads 1S" shows the same for Unibeads 1S as adsorptive material. Residues that a constant background (contamination), are marked with a "*c*", ones that represent a memory effect from a preceding sample are marked with an "*m*". Substances that are not detected regularly in ambient air samples or show poor measurement precision ≥ 10 % were excluded from the analysis ("not analysed"; n.a.). If no residue was detected or the detected residue was ≤ 0.01 %, a "not detected" (n.d.) is assigned to the respective substance.

Table S-1. List of detectable substances and blank residues. Descriptions are given in the text.

Class/Name	Formula	t_R [min]	bp [°C]	Residue HayeSep D	Residue Unibeads 1S
CFCs & HCFCs					
HCFC-22	$CHClF_2$	5.20	-41	n.d.	n.d.
CFC-115	$CClF_2CF_3$	4.48	-39	n.d.	n.d.
CFC-12	CF_2Cl_2	5.02	-30	n.d.	n.d.
HCFC-124	CHF_2CF_2Cl	6.85	-12	n.d.	n.d.
HCFC-142b	CH_3CClF_2	6.87	-10	n.d.	n.d.
HCFC-31	CH_2ClF	6.40	-9	n.a.	n.a.
CFC-114	$CClF_2CClF_2$	6.67	4	n.d.	n.d.
HCFC-133a	$C_2H_2ClF_3$	7.55	6	n.d.	n.d.
HCFC-21	$CHFCl_2$	7.32	9	n.d.	n.d.
CFC-11	$CFCl_3$	7.28	24	n.d.	n.d.
HCFC-141b	CH_3CCl_2F	8.42	32	n.d.	n.d.
HCFC-1121	CHClCFCl	8.05	35	n.a.	n.a.

Class/Name	Formula	t_R [min]	bp [°C]	Residue HayeSep D	Residue Unibeads 1S
HCFC-132b	$CH_2ClCClF_2$	9.08	46	n.d.	n.d.
CFC-113	CCl_2FCClF_2	8.45	48	0.2% (m)	n.d.
HCFC-225ca	$CF_3CF_2CHCl_2$	9.37	51	n.a.	n.a.
HCFC-225cb	$CClF_2CF_2CHClF$	9.57	56	n.a.	n.a.
CFC-112	$CFCl_2CFCl_2$	10.33	92	n.d.	n.d.
HCFC-131	CCl_3CH_2F	12.38	103	n.a.	n.a.
PFCs & HFCs					
HFC-23	CHF_3	3.01	-82	2.6% (c)	n.a.
HFC-41	CH_3F	4.38	-78	n.a.	n.a.
HFC-32	CH_2F_2	4.20	-52	n.d.	n.d.
HFC-125	CHF_2CF_3	4.87	-49	0.4% (c)	1.3% (c)
HFC-143a	CH_3CF_3	5.00	-48	n.d.	n.d.
HFC-161	C_2H_5F	6.85	-38	n.a.	n.a.
PFC-218	C_3F_8	4.02	-37	n.d.	n.d.
PFC-216	C_3F_6	4.58	-30	n.a.	n.a.
HFO-1234yf	$CHFCHCF_3$	5.72	-28	6.9% (c)	14.9% (c)
HFC-134a	CH_2FCF_3	5.92	-26	n.d.	n.d.
HFC-152a	CH_3CHF_2	6.53	-25	n.d.	n.d.
HFC-134	CHF_2CHF_2	6.32	-23	1.1% (c)	3.0% (c)
HFC-227ea	CF_3CHFCF_3	6.52	-16	n.d.	n.d.
HFO-1234ze	$CHFCHCF_3$	6.27	-16	n.d.	n.d.
PFC-318	$c\text{-}C_4F_8$	5.68	-6	n.d.	n.d.
HFC-236fa	$CF_3CH_2CF_3$	7.22	-1	n.d.	n.d.
HFC-329ccb	C_4HF_9	7.67	15	n.a.	n.a.
HFC-245fa	$CF_3CH_2CHF_2$	7.92	15	n.d.	n.d.
HFO-1233zd	$CHClCHCF_3$	7.82	19	n.a.	n.a.
HFC-356mff	$C_4H_4F_6$	8.35	25	n.a.	n.a.
HFC-365mfc	$CF_3CH_2CF_2CH_3$	9.27	40	n.a.	n.a.
Halons					
Halon-1301	$CBrF_3$	3.87	-58	n.d.	n.d.
Halon-1211	$CBrClF_2$	6.32	-4	n.d.	n.d.
Halon-1202	CF_2Br_2	7.45	23	n.a.	n.a.
Halon-2402	$CBrF_2CBrF_2$	8.53	47	n.d.	n.d.
Halon-2311	$CF_3CHBrCl$	9.30	50	n.a.	n.a.

Class/Name	Formula	t_R [min]	bp [°C]	Residue HayeSep D	Residue Unibeads 1S
Chloro-, Bromo- & Iodocarbons					
Chloromethane	CH_3Cl	6.02	-24	0.5% (c)	0.6% (c)
Bromomethane	CH_3Br	7.00	4	3.4% (c)	1.8% (c)
Chloroethane	C_2H_5Cl	7.92	12	25.5% (c)	8.6% (c)
Dichloromethane	CH_2Cl_2	8.17	40	0.4% (c, m)	0.2% (c)
Iodomethane	CH_3I	8.00	42	43.9% (c, m)	46.2% (c, m)
Trichloromethane	$CHCl_3$	8.92	61	1.4% (c, m)	0.7% (c, m)
Bromochloromethane	CH_2BrCl	9.03	68	n.d.	n.d.
Methyl chloroform	CH_3CCl_3	9.93	74	n.d.	n.d.
Tetrachloromethane	CCl_4	9.08	77	1.1% (m)	n.d.
Trichloroethene	C_2HCl_3	9.55	87	n.d.	n.d.
Bromodichloromethane	$CHBrCl_2$	10.10	90	n.d.	n.d.
Dibromomethane	CH_2Br_2	10.03	96	n.d.	n.d.
Dibromochloromethane	$CHBr_2Cl$	11.53	119	n.d.	n.d.
Tetrachloroethene	C_2Cl_4	10.62	121	23.9% (c, m)	5.2% (c, m)
Tribromomethane	$CHBr_3$	13.50	147	11.2% (m)	n.d.
Diiodomethane	CH_2I_2	15.00	181	n.a.	n.a.
Sulfur-containing and other halogenated compounds					
Sulfuryldifluoride	SO_2F_2	4.20	-55	n.d.	n.d.
Carbonyl sulfide	COS	3.77	-50	0.4% (c)	0.1% (c)
Chlorotrifluoroethylene	C_2F_3Cl	4.92	-28	n.a.	n.a.
Perfluorotetrahydrofuran	C_4F_8O	5.87	2	n.a.	n.a.
3-chloropentafluoropropene	CF_2CFCF_2Cl	8.07	8	n.d.	7.6% (c)
Desflurane	$CF_3CHFOCHF_2$	8.42	24	n.a.	n.a.
Carbon disulfide	CS_2	6.54	46	4.0% (c)	0.8% (c)
Isoflurane	$CHF_2OCHClCF_3$	9.83	49	n.a.	n.a.
Sevoflurane	$CF_3CF_3CHOCH_2F$	10.35	59	n.a.	n.a.

Class/Name	Formula	t_R [min]	bp [°C]	Residue HayeSep D	Residue Unibeads 1S
Hydrocarbons and Aldehydes					
Ethyne	C_2H_2	3.75	-81	0.3% (c)	1.4% (c)
Propene	C_3H_6	5.38	-48	35.2% (c)	28.5% (c)
Propane	C_3H_8	4.09	-42	0.4% (c)	0.1% (c)
Propyne	C_3H_4	7.17	-23	n.d.	n.d.
Formaldehyde	CH_2O	7.62	-19	n.a.	n.a.
Isobutane	C_4H_{10}	5.79	-13	0.7% (c)	1.0% (c)
Isobutene	C_4H_8	7.32	-7	n.d.	75.3% (c)
1-butene	C_4H_8	7.38	-6	n.a.	n.a.
1,3-butadiene	C_4H_6	7.32	-4	n.a.	n.a.
n-butane	C_4H_{10}	6.05	-1	0.3% (c)	0.1% (c)
trans-2-butene	C_4H_8	7.02	1	25.3% (c)	19.8% (c)
cis-2-butene	C_4H_8	7.24	4	n.a.	n.a.
Acetaldehyde	C_2H_4O	11.26	20	99.2% (c, m)	82.0% (c, m)
2-methylbutane	C_5H_{10}	7.40	28	0.4% (m)	0.2% (m)
Isoprene	C_5H_8	8.67	34	n.a.	n.a.
n-pentane	C_5H_{12}	7.57	36	0.7% (m)	0.3% (m)
trans-2-pentene	C_5H_{10}	8.47	36	n.d.	22.2% (c, m)
cis-2-pentene	C_5H_{10}	8.56	37	n.a.	n.a.
2-methylpentane	C_6H_{14}	8.61	60	0.8% (m)	1.0% (m)
3-methylpentane	C_6H_{14}	8.71	63	1.8% (m)	n.d.
n-hexane	C_6H_{14}	8.71	68	1.5% (c)	n.d.
Benzene	C_6H_6	11.00	80	2.5% (c)	5.2% (c)
Cyclohexane	c-C_6H_{12}	8.82	81	n.d.	n.d.
n-heptane	C_7H_{16}	10.06	98	23.1% (c, m)	4.0% (m)
Toluene	C_7H_8	14.52	111	17.4% (c, m)	9.8% (c, m)

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